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Randall K. Walters

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Bernard F. Engebos

ATMOSPHERIC SCIENCES RESEARCH OFFICE

WHITE SANDS MISSILE RANGE, NEW MEXICO

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ABSTRACT

An improved method to control error in the classical Runge-Kutta numerical integration scheme has been uncovered. The method is readily adaptable to the solutions of the differential equations of motion of an unguided rocket. This report presents the theoretical aspects behind this method and an evaluation of its efficiency.

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INTRODUCTION

Most mathematical models for the simulation of the trajectory of a ballistic rocket employ the Runge-Kutta numerical integration scheme with the extrapolation-to-zero-grid error control criterion of Richardson [1]. This criterion is based on a comparison of the results obtained by numerically integrating with step sizes of h and $\frac{h}{2}$. This involves evaluating the functional equations eleven times for a single integration step, seven of the evaluations being performed solely for the purpose of error control.

An alternate technique for error control was suggested by Earnest [2]. This report investigates Earnest's technique and compares the efficiency of this technique to that of Richardson.

DISCUSSION

Suppose one has a system of first-order ordinary differential equations of the form

$$\frac{dy_i}{dx} = y_i' = f_i\ (x,\ y_1,\ \ldots,\ y_N)\quad i = 1,\ \ldots,\ N \tag{1}$$

with initial conditions $y_i(x_0) = y_{i0}$, $i = 1, \ldots, N$. The Runge-Kutta fourth-order method is an algorithm designed to approximate the Taylor series expansions

$$y_i(x_0 + h) = y_{i0} + h\ y_{i0}' + \frac{h^2}{2!}\ y_{i0}'' + \ldots \tag{2}$$

of (1) and has the general form

$$y_i(x_0 + h) = y_{i0} + aK_{i0} + bK_{i1} + c\ K_{i2} + dK_{i3} \tag{3}$$

where

$$\begin{aligned}
K_{i0} &= hf_i(x_0,\ y_{10},\ \ldots,\ y_{N0}), \qquad i = 1,\ \ldots,\ N \\
K_{i1} &= hf_i(x_0 + lh,\ y_{10} + m\ K_{10},\ \ldots,\ y_{N0} + m\ K_{N0}) \\
K_{i2} &= hf_i(x_0 + nh,\ y_{10} + q\ K_{10} + r\ K_{11},\ \ldots,\ y_{N0} + q\ K_{N0} + r\ K_{N1}) \\
K_{i3} &= hf_i(x_0 + ph,\ y_{10} + v\ K_{10} + s\ K_{11} + t\ K_{12},\ \ldots).
\end{aligned} \tag{4}$$

For purposes of completeness a brief discussion of the determination of the above parameters is included in Appendix A; the reader is referred to [3] for a more thorough discussion.

THE ERROR CONTROL

1. Derivation

One assumes a truncation error estimate of (3) to be of the form

$$T_i = \alpha K_{i0} + \beta K_{i1} + \gamma K_{i2} + \delta K_{i3} + \varepsilon K_{i4}, \quad i = 1, \ldots, N \qquad (5)$$

where K_{i4} is K_{i0} of the next integration step. A reasonable truncation error estimate will be achieved if (5) reflects the magnitude of the fourth-order term of the Taylor series expansions of (1). This is accomplished by expanding (5) in a Taylor series and requiring the first three terms to be zero.

Similar to the procedure in Appendix A, one considers the case of one dependent variable; K_{i4} thus becomes

$$K_{i4} = K_4 = hf(x_0 + h,\ y_0 + a\,K_0 + b\,K_1 + c\,K_2 + d\,K_3) \qquad (6)$$

The error control is obtained from a Taylor series expansion of (6). For simplicity of notation, define operators D_4 and D_{41} by

$$D_4 = \frac{\partial}{\partial x} + (a + b + c + d) f_0 \frac{\partial}{\partial y}$$

and

$$\begin{aligned} D_{41} &= h \frac{\partial}{\partial x} + (a\,K_0 + b\,K_1 + c\,K_2 + d\,K_3) \frac{\partial}{\partial y} \\ &= h\,D_4 + [b(K_1 - hf_0) + c(K_2 - hf_0) + d(K_3 - hf_0)] \frac{\partial}{\partial y} \end{aligned}$$

In terms of operators D_1, D_2, and D_3 defined in Appendix A,

$$\begin{aligned} K_4 &= h\left[f + D_{41}\,f + \frac{D_{41}^2}{2!}\,f + \frac{D_{41}^3}{3!}\,f + \ldots\right]_{x = x_0} \\ &= h\{f + h\,D_4\,f + \frac{h^2}{2!}\,D_4^{\,2}\,f + h^2 f_y[bD_1 f + c\,D_2\,f + d\,D_3 f] \\ &\quad + \frac{h^3}{3!}\,D_4^{\,3}\,f + \frac{h^3}{2}\,f_y[bD_1^{\,2}\,f + c\,D_2^{\,2}\,f + d\,D_3^{\,2}\,f] \\ &\quad + h^3\,f_y^{\,2}\,[crD_1 f + d(sD_1 f + tD_2 f)] \\ &\quad + h^3\,D_4 f_y[bD_1 f + c\,D_2 f + dD_3 f]\}_{x = x_0} \end{aligned} \qquad (7)$$

Substituting (A9)* and (7) into (5) and equating the first three terms of the Taylor series expansion of (5) to zero yields the following four algebraic equations:

$$\alpha + \beta + \gamma + \delta + \varepsilon = 0$$

$$\beta m + \gamma n + \delta p + \varepsilon = 0$$

$$\beta m^2 + \gamma n^2 + \delta p^2 + \varepsilon = 0$$

$$\gamma rm + \delta(sm + tn) + \varepsilon(bm + cn + dp) = 0 \tag{8}$$

Since the four equations above involve five new parameters one may solve for them in terms of one of the new parameters. The general solution of (8) in terms of the parameter ε and the previously selected independent parameters is given in Table AI of Appendix A.

To gain more information about the error estimate, it is required that the fourth-order term of the Taylor series expansion of (5) match as closely as possible the corresponding fourth-order term of (A5). For this purpose, fitting coefficients are defined which express the difference between the coefficients of the corresponding fourth-order terms mentioned above. By using (7), (A9), (A10), (5), and (A5) these fitting coefficients are given by

$$F_1 = 1/6\ (\beta m^3 + \gamma n^3 + \delta p^3 + \varepsilon) - 1/24$$

$$F_2 = \gamma rmn + \delta p\ (sm + tn) + \varepsilon\ (bm + cn + dp) - 1/8 \tag{9}$$

$$F_3 = 1/2\ [\gamma rm^2 + \delta(sm^2 + tn^2) + \varepsilon\ (bm^2 + cn^2 + dp^2)] - 1/24$$

$$F_4 = \delta trm + \varepsilon[crm + d(sm + tn)] - 1/24.$$

The selected value of ε should be one which minimizes these fitting coefficients. Table AI includes the expression of these coefficients in terms of the previously chosen independent parameters.

From the Case II methods in Table AI, the choice of $t = 1$ yields the classical formulas of Runge while $t = 1 + \sqrt{1/2}$ yields the Runge-Kutta-Gill method.

Due to the simplicity of the truncation error estimate in Case II methods and from the form of the fitting coefficient, F_3, the choice of Case II methods with $\varepsilon = 1$ seems to be advantageous.

If (1) is a function of the independent variable only, the Case II methods reduce to Simpson's rule and the corresponding truncation error estimate clearly fails.

---

*(Ai) refers to (i) in Appendix A, i = 5,6,7,8,9,10.

2. Control of Step Size

To control the error in the numerical computation adequately it is desirable to have some criterion by which a decision may be made to alter the current integration step size. For a given numerical integration formula the control of the step size is based on comparisons of its associated truncation error estimates with the corresponding error limits for each variable. Therefore, by keeping the error limits constant, the truncation error will remain below a fixed bound, while using a fixed percentage of the current magnitude of each variable for the error limits keeps the relative error below a fixed bound.

In using the fixed percentage method, however, oscillating variables cause the calculations to bog down when these variables cross zero. Thus a weighted average of the previous magnitudes of the variables could be used as a basis for the error limits.

The truncation error estimate, T_i, can be used to circumvent the usual Richardson method of step size control. This is accomplished by assuming that the decision as to whether or not to increase the current step size is based on a prediction of what the truncation error estimates would be if a larger step size were used. Therefore, let h* be the larger step size and let T_i^* be the truncation error estimate using h*. By assuming that the truncation error estimate, T_i, is of order k and that the kth term of the Taylor series expansion of T_i dominates the expansion, one may approximate T_i^* by

$$T_i^* = \left(\frac{h^*}{h}\right)^k T_i .$$

In practice it is desirable to overestimate the factor T_i^* since this tends to reduce time-consuming premature increases in step size.

For a fourth-order method with $h^* = 2h$, $T_i^* = 32T_i$, let U_i be the predetermined bound for the truncation error estimate T_i. If $T_i > U_i$, $y_i(x_0 + h)$ is unacceptable. Therefore the step size h should be reduced and $y_i(x_0 + h)$ computed again using the smaller value of h. On the other hand, $T_i \leq U_i$ implies the integration is acceptable. If in addition, $T_i^* \leq U_i$, the truncation error generated by h* should be within an acceptable tolerance; thus, h* is used as the integration interval in the next integration.

Herein lies the true potential of the above technique - no additional functional evaluations were required beyond those of the numerical integration method itself.

APPLICATIONS AND CONCLUSIONS

The Runge-Kutta-Gill numerical integration scheme was incorporated into the six-degree-of-freedom mathematical ballistic models of Walter (4) and Duncan and Ensey (5). The coefficient $\varepsilon = 1$ was chosen for use in the estimate of truncation error. Several simulated trajectories were then computed for each of the following unguided rockets: the Aerobee 350 (a high-altitude research rocket), the BMTS (Ballistic Missile Target System), and the Athena (a reentry research rocket). The results of these simulations were compared to similar simulations using the Runge-Kutta-Gill integration scheme but with the extrapolation-to-the-zero-grid error control criterion.

The differences for each of the comparable simulations at burnout, at peak, and at impact were considered negligible (less than .1%). However, there was one notable difference - the mean processing time for a single trajectory simulation was reduced by 46% by incorporating the error technique as developed herein into the aforementioned ballistic models.

Since these ballistic models are to be used in real-time support of unguided rocket firings where time is so essential, there is a clear advantage in using the error check as developed herein to replace the currently used extrapolation-to-the-zero-grid method.

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APPENDIX A

THE GENERAL RUNGE-KUTTA METHOD

Suppose one has a system of first-order ordinary differential equations of the form

$$\frac{dy_i}{dx} = y_i' = f_i\ (x,\ y_i,\ \ldots,\ y_N)\ i = 1,\ \ldots,\ N \tag{A1}$$

with initial conditions $y_i\ (x_0) = y_{i0}$, $i = 1, \ldots, N$. The Runge-Kutta fourth-order method is an algorithm designed to approximate the Taylor series expansions

$$y_i\ (x_0 + h) = y_{i0} + h\ y_{i0}' + \frac{h^2}{2!} y_{i0}'' + \ldots \tag{A2}$$

of (A1) and has the general form

$$y_i\ (x_0 + h) = y_{i0} + aK_{i0} + bK_{i1} + c\ K_{i2} + dK_{i3} \tag{A3}$$

where

$$K_{i0} = hf_i(x_0,\ y_{10},\ \ldots,\ y_{N0}) \qquad i = 1,\ \ldots,\ N$$

$$K_{i1} = hf_i(x_0 + lh,\ y_{10} + m\ K_{10},\ \ldots,\ y_{N0} + m\ K_{N0}) \tag{A4}$$

$$K_{i2} = hf_i(x_0 + nh,\ y_{10} + q\ K_{10} + r\ K_{11},\ \ldots,\ y_{N0} + q\ K_{N0} + r\ K_{N1})$$

$$K_{i3} = hf_i(x_0 + ph,\ y_{10} + v\ K_{10} + s\ K_{11} + t\ K_{12},\ \ldots).$$

To reduce somewhat the unwieldy nature of the notation, one requires that (A1) be a function of one dependent variable, and defines $D = \frac{\partial}{\partial x} + f\frac{\partial}{\partial y}$ and $f_y = \frac{\partial f}{\partial y}$. The Taylor series solutions of A1 can now be written as

$$y(x_0 + h) = y_0 + [hf + \frac{h^2}{2!}\ Df + \frac{h^3}{3!}\ (D^2f + f_y\ Df) \tag{A5}$$

$$+ \frac{h^4}{4!}\ (D^3f + f_y\ D^2f + f_h{}^2\ Df + 3Df\ Df_y) + \ldots]_{x = x_0}$$

while the fourth-order Runge-Kutta method takes on the following form:

$$y(x_0 + h) = y_0 + a\ K_0 + bK_1 + c\ K_2 + d\ K_3 \tag{A6}$$

where

$$K_0 = hf(x_0,\ y_0)$$

$$K_1 = hf(x_0 + 1h,\ y_0 + m\,K_0)$$

$$K_2 = hf(x_0 + nh,\ y_0 + q\,K_0 + rK_1)$$

$$K_3 = hf(x_0 + ph,\ y_0 + v\,K_0 + s\,K_1 + tK_2). \tag{A7}$$

For the Taylor series expansion of A7 one defines the following operators:

$$D_1 = 1\,\frac{\partial}{\partial x} + mf_0\,\frac{\partial}{\partial y}$$

$$D_2 = n\,\frac{\partial}{\partial x} + (q + r)\,f_0\,\frac{\partial}{\partial y}$$

$$D_3 = p\,\frac{\partial}{\partial x} + (v + s + t)f_0\,\frac{\partial}{\partial y} \tag{A8}$$

where $f_0 = f(x_0)$. Using A8, the expansions of K_0, K_1, K_2, and K_3 are

$$K_1 = hf_0$$

$$K_2 = h\,[f + h\,D_1\,f + \frac{h^2}{2!}\,D_1^{\,2}\,f + \frac{h^3}{3!}\,D_1^{\,3}\,f + \frac{h^4}{4!}\,D_1^{\,4}\,f + \ldots]_{x\,=\,x_0}$$

$$\begin{aligned}
K_3 = h\,\{&f + h\,D_2 f + \frac{h}{2!}\,D_2^{\,2}\,f + \frac{h^3}{3!}\,D_2^{\,3}\,f + \frac{h^4}{4!}\,D_2^{\,4}\,f + \ldots \\
&+ h^2 r[f_y D_1 f + \frac{h}{2!}\,f_y\,D_1^{\,2}\,f + h\,D_1\,f\,D_2 f_y + \frac{h^2}{3!}\,f_y\,D_1^{\,3}\,f \\
&+ \frac{h^2}{2}\,D_1^{\,2}\,f\,D_2 f_y + \frac{h^2}{2!}\,r\,f_{yy}\,(D_1\,f)^2 + \frac{h^2}{2!}\,D_1 f\,D_2^{\,2}\,f_y]\}_{x\,=\,x_0}
\end{aligned}$$

$$\begin{aligned}
K_4 = h\,\{&f + h\,D_3 f + h^2\,f_y\,[s(D_1 f + \frac{h}{2}\,D_1^{\,2}\,f + \frac{h}{3!}\,D_1^{\,3}\,f + \ldots) \\
&+ t(D_2\,f + hr\,f_y\,D_1 f + \frac{h}{2}\,D_2^{\,2}\,f + \frac{h^2}{2}\,r\,f_y\,D_1^{\,2}\,f + h^2\,D_1\,f\,D_2\,f_y + \frac{h^2}{3!}\,D_2^{\,3} f \\
&+ \frac{1}{2!}\,(h^2\,D_3^{\,2}\,f + 2h^3\,D_3\,f_y\,[s(D_1\,f + \frac{h}{2}\,D_1^{\,2}\,f + \ldots) + t(D_2 f + \frac{h}{2}\,D_2^{\,2}\,f \\
&+ hr\,f_y\,D_1 f + \ldots)] + h^4\,f_{yy}[s^2(D_1 f)^2 + 2\,st\,D_1 f\,D_2\,f \\
&+ t^2\,(D_2\,f)^2 + \ldots]) + \frac{1}{3!}\,(h^3\,D_3^{\,3}\,f + 3h^4\,D_3^{\,2}\,f_y\,[s\,D_1 f + t\,D_2\,f + \ldots]) \\
&+ \frac{1}{4!}\,(h^4\,D_3^{\,4}\,f + \ldots) + \ldots\}_{x\,=\,x_0}.
\end{aligned} \tag{A9}$$

By requiring that the Runge-Kutta method be independent of the choice of the function f, one obtains from (A8)

$$1 = m,\ n = q + r,\ p = v + s + t$$

$$\text{i.e. } D_1 = mD,\ D_2 = nD,\ D_3 = pD. \qquad \text{(A10)}$$

Substitution of (A10) into (A9), and then into (A6), and equating the resulting set of equations term-by-term to the Taylor series expansion (A5) yields the following set of eight algebraic equations in ten unknowns.

$$a + b + c + d = 1 \qquad crm + d(sm + tn) = 1/6$$

$$bm + cn + dp = 1/2 \qquad crm^2 + d(sm^2 + tn^2) = 1/2$$

$$bm^2 + cn^2 + dp^2 = 1/3 \qquad crmn + dp(sm + tn) = 1/8$$

$$bm^3 + cn^3 + dp^3 = 1/4 \qquad dtrm = 1/24 \qquad \text{(A11)}$$

Table AI lists the general solution of the equations in (A11) in terms of the parameters m and n and several special cases of the solution which result from certain sets of equations in (A11) being linearly dependent for particular values of m and n.

TABLE AI
SOLUTIONS OF EQUATIONS

Case / Variable	I	II	III	IV
m	m	$1/2$	1	$1/2$
n	n	$1/2$	$1/2$	0
p	1	1	1	1
r	$\frac{n(m-n)}{2m(2m-1)}$	$\frac{1}{2t}$	$\frac{1}{8}$	$\frac{1}{2t}$
s	$\frac{(1-m)(m-4n^2+5n-2)}{2m(n-m)(6mn-4m-4n+3)}$	$1-t$	$-\frac{t}{4}$	$\frac{3}{2}$
t	$\frac{(1-2m)(1-m)(1-n)}{n(n-m)(6mn-4m-4n+3)}$	t	t	t
a	$\frac{6mn-2m-2n+1}{12mn}$	$\frac{1}{6}$	$\frac{1}{6}$	$\frac{1-t}{6}$
b	$\frac{2n-1}{12m(n-m)(1-m)}$	$\frac{2-t}{3}$	$\frac{t-2}{6t}$	$\frac{2}{3}$
c	$\frac{2m-1}{12n(m-n)(1-n)}$	$\frac{t}{3}$	$\frac{2}{3}$	$\frac{t}{6}$
d	$\frac{6mn-4m-4n+3}{12(1-m)(1-n)}$	$\frac{1}{6}$	$\frac{1}{3t}$	$\frac{1}{6}$
α	$\frac{\varepsilon(2m-1)(2n-1)}{2mn}$	0	0	$-\varepsilon t$
β	$-\frac{\varepsilon(2m-1)(2n-1)}{2m(n-m)(1-m)}$	0	$\frac{\varepsilon(2-t)}{t}$	0
γ	$\frac{\varepsilon(2m-1)(2n-1)}{2n(n-m)(1-n)}$	0	0	εt
δ	$-\frac{\varepsilon(6mn-4m-4n+3)}{2(1-m)(1-n)}$	$-\varepsilon$	$-\frac{2\varepsilon}{t}$	$-\varepsilon$
ε	ε	ε	ε	ε
F_1	$-\frac{\varepsilon(2m-1)(2n-1)}{12}-\frac{1}{24}$	$-\frac{1}{24}$	$-\frac{1}{24}$	$-\frac{1}{24}$
F_2	$\frac{\varepsilon(2n-1)}{4}-\frac{1}{8}$	$-\frac{1}{8}$	$-\frac{1}{8}$	$-\frac{2\varepsilon+1}{8}$
F_3	$\frac{\varepsilon(3m-1)}{12}-\frac{1}{24}$	$\frac{\varepsilon-1}{24}$	$\frac{4\varepsilon-1}{24}$	$\frac{\varepsilon-1}{24}$
F_4	$\frac{\varepsilon}{12}-\frac{1}{24}$	$-\frac{2\varepsilon+1}{24}$	$-\frac{2\varepsilon+1}{24}$	$-\frac{2\varepsilon+1}{24}$

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13. ABSTRACT

An improved method to control error in the classical Runge-Kutta numerical integration scheme has been uncovered. The method is readily adaptable to the solutions of the differential equations of motion of an unguided rocket. This report presents the theoretical aspects behind this method and an evaluation of its efficiency.

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